A NEW METHOD FOR CONDITIONING STOCHASTIC GROUNDWATER FLOW MODELS IN FRACTURED MEDIA

A. Milne[1], K. A. Cliffe[2], D. Holton[3], P. Houston[4], C. P. Jackson[5], S.Joyce[6]

ABSTRACT

Many geological formations consist of crystalline rocks that have very low matrix permeability but allow flow through an interconnected network of fractures. Understanding the flow of groundwater through such rocks is important in considering disposal of radioactive waste in underground repositories. A specific area of interest is the conditioning of fracture transmissivities on measured values of pressure in these formations. This is the process where the values of fracture transmissivities in a model are adjusted to obtain a good fit of the calculated pressures to measured pressure values. While there are existing methods to condition transmissivity fields on transmissivity, pressure and flow measurements for a continuous porous medium there is little literature on conditioning fracture networks. Conditioning fracture transmissivities on pressure or flow values is a complex problem because the measurements are not linearly related to the fracture transmissivities and they are also dependent on all the fracture transmissivities in the network.
We present a new method for conditioning fracture transmissivities on measured pressure values based on the calculation of certain basis vectors; each basis vector represents the change to the log transmissivity of the fractures in the network that results in a unit increase in the pressure at one measurement point whilst keeping the pressure at the remaining measurement points constant. The fracture transmissivities are updated by adding a linear combination of basis vectors and coefficients, where the coefficients are obtained by minimizing an error function. A mathematical summary of the method is given. This algorithm is implemented in the existing finite element code ConnectFlow developed and marketed by Serco Technical Services, which models groundwater flow in a fracture network. Results of the conditioning are shown for a number of simple test problems as well as for a realistic large scale test case.

Key words: fracture network, model calibration, groundwater flow, finite element method.

[1,2,4]School of Mathematical Sciences, University of Nottingham, Nottingham, UK
[1]pmxam3@nottingham.ac.uk, [2]Andrew.Cliffe@nottingham.ac.uk, [4]Paul.Houston@nottingham.ac.uk

[3,5,6]Serco Technical Services, Harwell, UK
[3]David.Holton@serco.com, [5]CPeter.Jackson@sercoassurance.com, [6]Steve.Joyce@serco.com

1 – INTRODUCTION

In many countries the civil nuclear industry is investigating the feasibility of long term disposal of radioactive waste in repositories located deep in geological formations consisting of mostly crystalline rock. The main transport route to the surface environment for leached waste would be through groundwater flow. Crystalline rock has a very low permeability and is frequently fractured. In this setting, groundwater flow occurs through the network of fractures, which are represented as planar features in numerical models (*Hartley* [9]). The network is characterised by the properties of the fractures, the density of the fractures, their size, orientation and transmissivity. The transmissivity of a fracture is defined as the rate of groundwater flow per unit pressure gradient. It thus gives a measure of the ease with which groundwater can pass through a material (a fracture in our case). The fracture transmissivity is proportional to the cube of the fracture aperture (width) (*Zimmerman and Bodvarsson* [21]). In a problem of practical relevance, there are generally too many fractures for all of their properties to be measured. To remedy this problem a stochastic approach can be exploited; here distributions of fracture properties are inferred from field measurements and are subject to uncertainty (

Bonnet et al. [1], *Marrett* [13], *Snow* [20]). Realizations of the fractures can be generated in a volume of rock with the fracture properties sampled from distributions consistent with the observed measurements. Fractures with known properties can also be included deterministically in a model of this type. The groundwater flow equation can be used to calculate the pressure in a fracture, and at fracture intersections there are boundary conditions representing conservation of mass and continuity of pressure (see *Hartley* [9] for details).

Finite element techniques have been developed to solve groundwater flow and transport problems in single fractures (*Grisak and Pickens* [8], *Huyakorn et al*.[11]). In our work the complete fracture network is discretized using the finite element code ConnectFlow [9] which is a software package that models flow and transport through fractured rock. The models are based on a direct representation of the discrete fractures making up the flow-conducting network. ConnectFlow generates representations of fractures; these can be either stochastic or deterministic. The software is based on a finite-element method that allows the flow through many thousands of fractures to be calculated.

When studying fracture networks it is common to use more than one realization of the network due to uncertainties in the fracture properties. In this setting, the geometry of the fractures is sampled from various distributions; thus each realization will have a different fracture geometry.

Due to the uncertainties involved in the fracture geometry, hydraulic properties and boundary conditions assigned to a realization, it is important for each realization to be as accurate as possible. Calibration is the process of modifying the input parameters to a model until the output from the model matches observed data. In this article, we wish to calibrate each realization of a fracture network to ensure that the output matches measured values. Each realization should be calibrated using as much available data as possible. Model parameters are generally conditioned on measured values such as pressures and flow rates.

Our proposed conditioning method considers one realization where the geometry of the fracture network is assumed fixed. In particular, only fracture transmissivities are adjusted to fit measured pressures, while keeping the position and orientation of each fracture fixed. In the event that the conditioning method does not produce a good fit to the measured values, then this may be an indication that the underlying fracture geometry is incorrect.

Our conditioning method shares some of the techniques used in inverse problems in hydrology (*Neuman* [16] *Neuman* [17], *Neuman et al*.[18], *Clifton and Neuman* [5] *Carrera, Alcolea et al.* [2] *Medina and Carrera* [14], *Dai and Samper* [7], *Hernandez et al.* [10]).

This article is structured as follows. In section 2, we provide a mathematical description of our method for conditioning fracture transmissivities on measured pressure values. In section 3, we show our results obtained from testing our code on four simple test cases. Section 4 shows results from conditioning fracture transmissivities on pressure measurements for a test case based on data from a real site. Section 5 provides a summary and draws conclusions from testing the proposed conditioning algorithm on the available test cases.

2 – MATHEMATICAL DESCRIPTION OF THE NEW METHOD FOR CONDITIONING STOCHASTIC GROUNDWATER FLOW MODELS IN FRACTURED MEDIA

Cliffe and Jackson [4; 12] proposed a method for conditioning continuous porous medium models on pressure measurements. In this section, we generalise this approach to condition fracture transmissivities on pressure measurements in a fracture network. Here, the rock is assumed to be impermeable and the only route taken by groundwater is through a network of fractures. To our knowledge, there are no existing methods that will condition fracture transmissivities in a discrete fracture network based on measured pressures.

The proposed conditioning method conditions fracture transmissivities on measured pressures at the intersection between a borehole and a fracture where the pumping rate of the borehole is specified. A borehole is a well of small radius that has been drilled into the rock. Boreholes can be pumped to create a flow or they are non-pumping. Our method is based on the calculation of certain basis vectors; each basis vector represents the change to the log transmissivity of the fractures in the network that results in a unit increase in the pressure at one measurement point whilst keeping the pressure at the remaining measurement points constant. The basic approach taken to update fracture transmissivity values to agree with measured pressure values is as follows. A simulation is run with an initial distribution of unconditioned fracture transmissivities. These fracture transmissivities are the parameters of our model which we wish to change. When there is a small variance in the values of fracture transmissivities, pressure measurements provide linear constraints on perturbations in fracture transmissivities. This

allows us to condition the fracture transmissivities directly by multiplying each basis vector by a given coefficient and adding a linear combination of the resulting vectors to the unconditioned transmissivities. The coefficients are the difference between the computed and measured pressures. The assumption of a linear relationship between perturbations in fracture transmissivities and pressure measurements allows basis vectors to be calculated where one basis vector corresponds to each measured pressure value. The basis vectors are dependent on the sensitivities of the fracture transmissivities. The sensitivity is the derivative of a measured pressure value with respect to a fracture transmissivity. Thus, it tells us how much influence the change in a fracture transmissivity will have on the measured pressure at a given point. However, we are interested in the more physically realistic case of when the variance in the fracture transmissivities is large. Here, we use the same basis vectors but the coefficients are determined by minimising an error function. Thereby, the conditioning will proceed iteratively, while the fracture transmissivities are updated until the error function has reached a suitable convergence criterion. The error function takes into account the difference between measured and calculated (from our simulation) pressure values. The number of coefficients in the model is equal to the number of measurement points. Thus, for large fracture networks, the number of model parameters is much less than the total number of fracture transmissivity values.
One of the key steps in the conditioning procedure is the calculation of the sensitivities. We require the sensitivity value of each measurement value with respect to every fracture transmissivity. To this end, adjoint methods can be used to calculate the desired sensitivities. Indeed, it is well known that adjoint methods are advantageous when the number of observation points is less than the number of parameters. Here, we are conditioning large fracture networks containing hundreds of fractures on a small number of measured pressure values and thus the number of parameters is much greater than the observation points; thereby, the adjoint method will be very efficient for this case. *Cirpka and Kitandis* [3] have used an adjoint method to calculate sensitivities of tracer data and pressure measurements. Non-linear minimisation of the error function is performed using the Levenberg Marquardt method. This is an efficient method for nonlinear optimisation (*Cooley* [6] and *Press et al.* [19]).
Firstly in section 2.1, we consider the case in which the variability is small and we introduce the relevant equations needed to produce conditioned fracture log transmissivities. In section 2.2, we consider the case of conditioning on pressure measurements when the variability is large; this involves the minimization of a corresponding error function.

2.1 – CONDITIONING ON PRESSURE MEASUREMENTS WHEN VARIABILITY IS SMALL

The material in this section is based on a conditioning method proposed by *Cliffe and Jackson* [4; 12] where an isotropic transmissivity field was conditioned on pressure measurements in a continuous porous medium. We extend this analysis so that it is applicable to a fracture network.
To this end, we consider the model of a fracture network where the transmissivity T is assumed to be constant on each fracture; correspondingly, the log transmissivity $X = \log_{10} T$ will also be constant on each fracture.
We define the vector $\mathbf{X}$ to contain the values of the log transmissivities X of the n fractures in the fracture network, i.e.,

$$\mathbf{X} = \begin{pmatrix} X_1 \\ \cdots \\ \cdots \\ X_n \end{pmatrix}. \tag{1}$$

Cliffe and Jackson [4; 12] showed that the conditioned realizations $\mathbf{X^C}$ of $\mathbf{X}$ are given by adding the product of basis vectors $\mathbf{W}$ and the vector of coefficients $\boldsymbol{\delta}\mathbf{P}$ to unconditioned fracture log transmissivities $\mathbf{X^U}$

$$\mathbf{X^C} = \mathbf{X^U} + \mathbf{W}\left(\boldsymbol{\delta}\mathbf{P}\right), \tag{2}$$

where $\mathbf{\delta P}$ contains the difference between measured pressure P_{meas} and calculated pressure P_{calc} at the m measurement points. That is

$$\mathbf{\delta P} = \begin{pmatrix} P_{\text{meas}}(1) - P_{\text{calc}}(1) \\ \dots \\ \dots \\ P_{\text{meas}}(m) - P_{\text{calc}}(m) \end{pmatrix}. \tag{3}$$

The matrix $\mathbf{W}$ contains the m basis vectors associated with each of the measurement points and as shown by *Cliffe and Jackson* [4; 12] is obtained by solving the system

$$\left(\mathbf{LCL^T}\right)\mathbf{W^T} = \mathbf{LC}. \tag{4}$$

The matrix $\mathbf{L}$ is known as the sensitivity matrix while the covariance matrix $\mathbf{C}$ represents the correlation of the fracture transmissivities in the network. For our work we have set $\mathbf{C}$ equal to the identity matrix, i.e., this assumes that the transmissivities of the fractures in the network are uncorrelated.

We consider the case where the sensitivity matrix $\mathbf{L}$ contains pressure measurements only. It represents the linear relationship between the values of $\mathbf{X}$ on n fractures and the measured values of pressure for small variability and small deviations of pressure from the mean pressure field. To calculate the entries of $\mathbf{L} = \left\{L_{ij}\right\}$, $i = 1,\dots,m$, $j = 1,\dots,n$ for the case of a fracture network we define the sensitivity as

$$L_{ij} = \frac{dP_B\left(m_i\right)}{dX_j}, \quad i = 1,\dots,m, \; j = 1,\dots,n, \tag{5}$$

where P_B is the borehole pressure measured at the ith measurement point m_i. The borehole pressure is the sum of the residual pressure P^R and a flow term at the borehole, namely,

$$P_B = P^R + \frac{Q}{T_f \kappa}, \tag{6}$$

where T_f is the fracture transmissivity, Q is the groundwater flow rate and κ is a geometric constant that takes into account the difference between the borehole pressure and the computed finite element pressure at a well due to the scale of the finite element discretisation.

We also define the consequence G at a measurement point m_i, $1 \le i \le m$, to be the difference between the calculated borehole pressure and the measured pressure

$$G\left(P, X\right) = P_B - P_{\text{meas}}. \tag{7}$$

There are two terms needed to calculate the entries in the sensitivity matrix defined in (5). For a fracture f, $1 \le f \le n$,

$$L_{if} = \int_f \nabla\theta \frac{1}{\rho g} \frac{\partial T_f}{\partial X_f} \nabla P + \frac{\partial}{\partial X_f}\left(\frac{Q}{T_j \kappa}\right), \tag{8}$$

where the first term corresponds to

$$\int_f \nabla\theta \frac{1}{\rho g}\frac{\partial T_f}{\partial X_f}\nabla P = \int_f \nabla\theta \frac{T_f \log_e 10}{\rho g}\nabla P \ , \tag{9}$$

and ∇P is the gradient of the pressure on the fracture f, $\nabla\theta$ is the gradient of the adjoint vector on the fracture f, ρ is the water density and g is gravitational acceleration.
The second term is calculated by differentiating (7) with respect to $X_f = \log_{10} T_f$, for a single fracture it corresponds to

$$\frac{\partial}{\partial X_f}\left(\frac{Q}{T_j\kappa}\right) = -\frac{Q\delta_{fj}\log_{10} e}{T_j\kappa}, \tag{10}$$

where $j = 1,...,n$, and δ is the Kronecker delta function. The integral in (9) can be calculated using a numerical quadrature technique while (10) may be easily evaluated. Details on the derivation of the sensitivity terms for a fracture network can be found in *Milne* [15].

2.2 – CONDITIONING ON PRESSURE MEASUREMENTS WHEN VARIABILITY IS LARGE

So far we have only considered the case of small variability in fracture transmissivities and small deviations of the pressure from the mean pressure field. In general, such assumptions cannot represent natural fracture networks accurately. Thereby, we now consider the situation of large variability and large deviations of the pressure from the mean pressure field. Here, the unconditioned transmissivity values and basis vectors $\mathbf{W}_i$ are computed as before. The log of the unconditioned fracture transmissivities is denoted by $\mathbf{X_0}$ and an update to the log transmissivities is evaluated assuming the following relationship suggested in *Cliffe and Jackson* [12]

$$\mathbf{X} = \mathbf{X_0} + \sum_{i=1}^{m}\alpha_i \mathbf{W}_i \ , \tag{11}$$

where α_i are coefficients which we wish to determine. Initially, the values of α are set to zero. The coefficients α_i are chosen so that they minimise an error function $E(\alpha)$ defined as the weighted sum of the consequences defined in (7), namely,

$$E(\alpha) = \sum_{i=1}^{N}\frac{G_i\left(P^R, \boldsymbol{\alpha}\right)^2}{\sigma_i^2}, \tag{12}$$

where σ_i is a weight corresponding to the estimated experimental error in the measurement of the pressure at measurement point i.
Our fracture network model depends non-linearly on $\boldsymbol{\alpha}$, thereby minimisation of (12) will proceed in an iterative manner. There are many different algorithms for non-linear minimisation and we exploit the Levenberg-Marquardt method to efficiently minimise $E(\boldsymbol{\alpha})$. For a concise description of the Levenberg Marquardt method, see *Press et al.* [19].
The Levenberg-Marquardt algorithm requires the derivative

$$\beta_k = \frac{\partial E}{\partial \alpha_k} = \sum_{i=1}^{m} \frac{2G_i}{\sigma_i^2} \frac{\partial G_i}{\partial \alpha_k}, \qquad k = 1,...,N \ , \tag{13}$$

and

$$\gamma_{kl} = \frac{\partial^2 E}{\partial \alpha_k \partial \alpha_l} = \sum_{i=1}^{N} \frac{1}{\sigma^2} \left[\frac{\partial G_i}{\partial \alpha_k} \frac{\partial G_i}{\partial \alpha_l} \right], \qquad l = 1,...,N \ , \tag{14}$$

for the m measurement points. The term $\frac{\partial G_i}{\partial \alpha_f}$ can be calculated by using the chain rule with the sensitivity values. The increments of the coefficients $\delta\alpha$ are calculated by solving the system

$$\sum_{l,k=1}^{N} \gamma'_{kl} \delta\alpha = \beta_k \ , \tag{15}$$

where

$$\begin{cases} \gamma'_{jk} = \gamma \left(1 + \lambda\right), & j = k \ , \\ \gamma'_{jk} = \gamma, & j \neq k \ , \end{cases} \tag{16}$$

and λ is a parameter initially set to a small value which will change by a factor of ten with each iteration. It controls whether the Levenberg Marquardt corresponds to a steepest decent method or a Newton method for the minimisation at each iteration. There are two different approaches that can be taken for the minimisation. One in which the derivatives (13) and (14) are updated with each iteration and one in which they are not. We use the terminology updating in this article to mean that the derivatives (13) and (14) are updated with each iteration. The minimisation algorithm is summarised as follows

1. Compute the initial log transmissivity field $\mathbf{X_0}$, and calculate an initial error from (12).
2. Calculate the sensitivities using (9) and (10).
3. Calculate the basis vectors using (4).
4. Select an initial guess for the coefficients α .
5. Update $\mathbf{X}$ using (11).
6. Re-calculate pressures with new $\mathbf{X}$ value.
7. If required, update the new derivatives in (13) and (14). Recalculate γ and β .
8. Calculate new increment for the coefficients $\delta\alpha$ from (15).
9. If error (12) has converged then stop. If error has not been reduced then increase λ by a factor of 10 and return to 6. If the error has been reduced then decrease λ by a factor of 10 and update $X\left(\alpha\right)$ to $X\left(\alpha + \delta\alpha\right)$ and return to 6.

3 – SIMPLE TEST CASES

The conditioning method described above was implemented in ConnectFlow, an existing finite element code. Our conditioning method was initially tested on four different test cases. These test cases have deterministically placed fractures with simple fracture geometry. The problem domain is the cube $10\text{m} \times 10\text{m} \times 10\text{m}$. Boundary conditions are defined on the cube faces as either a pressure or flux boundary condition.

In these simple test cases a specified value of the transmissivity that the solution should converge to is known, which we call the target transmissivity. Here, we perturb the target transmissivity, and then determine the conditioned transmissivities that lead to the measured pressure values at given measurement points. Each test case was conditioned separately with and without updating.

Figure 1 shows the domains of the simple test cases used. Test case 1 and 2 share the same problem domain; here a borehole intersects a single fracture as can be seen in Figure 1(a). In test case 1 there is a constant flux of $1e^{-7}m^2/s$ assigned to the west face of the cubic domain (far left in Figure 1(a)) and a constant pressure value of 0Pa on the east face as boundary conditions. The borehole is a non-pumping borehole and thus has no flux associated with it.

The boundary conditions of test case 2 differ from test case 1. In this case, the borehole is a pumping borehole with a flux of $1e^{-5}m^3/s$ and there is a constant pressure of 0Pa on all of the faces of the cubic domain that are in contact with the fracture.

The domain of test case 3 is shown in Figure 1(b); here, three unconnected fractures each intersect a borehole. There is a specified flux of $1e^{-5}m^3/s$ on each borehole. The pressure is set to 0Pa on the north, south, east and west faces of the domain. Three individual borehole intersections are used on each fracture in test case 3 to approximate a single borehole intersecting all three fractures.

Test case 4 is the first test case where the fractures are connected. Figure 1(c) shows the 3 fractures with a borehole intersecting the fracture in contact with the west face and another borehole intersecting the fracture in contact with the east face. These boreholes are non-pumping boreholes. There is a pressure boundary condition of 0Pa on the east face, and a flux boundary condition of $1e^{-7}m^3/s$ on the west face.

To test the conditioning method we used initial fracture transmissivities up to 3 orders of magnitude different from the target transmissivities for the test cases. Table 1 shows the number of iterations required to converge to the target transmissivity of $1e^{-6}m^2/s$ for test case 1 and 2. These test cases were conditioned separately with and without updating. The number of iterations required for the error measure (12) to converge to a value less than 1 are shown for both updating options with the iterations required without updating shown in brackets. An error measure less than 1 signifies a good agreement in the measured and calculated pressures. In fact, some of the initial error measures used in this paper are of order 1^{10}. It can be seen that when updating is used the error converges with a respectable number of iterations for both test cases. However, we observe that the convergence of the algorithm may be adversely affected when no updating is employed. Indeed, in this case, the solution will converge for both test cases for initial transmissivity values smaller than the target transmissivity, but typically require a large number of iterations. Test case 1 fails to converge for an initial transmissivity of $1.1e^{-3}m^2/s$ and larger. Test case 2 fails to converge for larger initial transmissivity values than the target transmissivity.

Table 2 shows the number of iterations required to converge to the target transmissivities of $1e^{-6}m^2/s$, $2e^{-6}m^2/s$ and $3e^{-6}m^2/s$ for test case 3 and 4. Again, when using updating for these test cases the error converges in a relatively small number of iterations. When no updating is employed, test case 3 converges for values of initial transmissivity smaller than the target transmissivity but requires a large number of iterations. It fails to converge with initial transmissivity values of $1.1e^{-3}m^2/s$, $2.1e^{-3}m^2/s$, $3.1e^{-3}m^2/s$ and larger. Test case 4 converged for all of the initial transmissivities but needed more iterations for all initial transmissivities when conditioning was employed without updating as compared to when updating was exploited.

We conclude that the updating procedure is necessary for practical problems and can produce converged solutions in a small number of iterations for simple test cases.

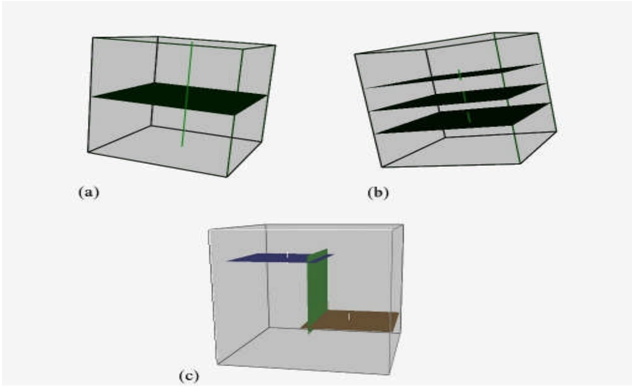

Figure 1. The cubic domains of (a) test cases 1 and 2 with a borehole intersecting a single fracture (b) test case 3 with 3 unconnected fractures each intersecting a separate borehole (c) test case 4 with 3 connected fractures and 2 of the planes intersecting separate boreholes.

Initial Transmissivity (m^2/s)	Number of iterations to convergence for test case 1	Number of iterations to convergence for test case 2
1.1e-2	15 (NC)	15 (NC)
1.1e-3	13 (NC)	13 (NC)
1.1e-4	11 (22)	11 (NC)
1.1e-5	9 (15)	9 (NC)
1.1e-6	2 (3)	3 (8)
1.1e-7	6 (92)	6 (94)
1.1e-8	8 (1004)	8 (1043)

Table 1. Number of iterations taken to converge to the measured pressures corresponding to a transmissivity of $1e^{-6}m^2/s$ for different initial transmissivity values for test case 1 and 2. Iteration values without brackets are from when updating was used and values in brackets are from when no updating was used. NC denotes that the error measure did not converge.

Initial Transmissivity (m^2/s)	Number of iterations to convergence for test case 3	Number of iterations to convergence for test case 4
1.1e-2, 2.1e-2, 3.1e-2	15 (NC)	19 (38)
1.1e-3, 2.1e-3, 3.1e-3	13 (NC)	19 (33)
1.1e-4, 2.1e-4, 3.1e-4	11 (26)	17 (24)
1.1e-5, 2.1e-5, 3.1e-5	9 (19)	10 (17)
1.1e-6, 2.1e-6, 3.1e-6	3 (8)	2 (3)
1.1e-7, 2.1e-7, 3.1e-7	6 (74)	6 (106)
1.1e-8, 2.1e-8, 3.1e-8	8 (927)	8 (1205)

Table 2. Number of iterations taken to converge to the measured pressures corresponding to a transmissivity of $1e^{-6}m^2/s$**,** $2e^{-6}m^2/s$, $3e^{-6}m^2/s$ for different initial transmissivity values for test case 3 and 4. Iteration values without brackets are from when updating was used and values in brackets are from when no updating was used. NC denotes that the error measure did not converge.

4 – REALISTIC TEST CASE

In this section we consider a fracture network based on data from a real site; see Figure 2. Here, there are 9 non-pumping boreholes that intersect given fractures in the domain. This test case represents a subset of the fractures at the site. This subset contains 501 fractures which are defined deterministically. Measured pressure values are obtained at measurement points at each of the 9 boreholes. The initial values of the fracture transmissivities are based on separate test site data from the pressure measurements. We will refer to the pressure values at the measurement points obtained from the initial fracture transmissivities as the unconditioned pressures.
We firstly consider conditioning the fracture transmissivities on “artificial” pressure measurements. These pressure measurements correspond to pressure values obtained at measurement points as a solution from a set of randomly generated fracture transmissivities. Thus, we know that a set of fracture transmissivity values exists which will produce our “artificial” pressure measurements at the measurement points.
After conditioning on “artificial” pressure measurements we condition the fracture transmissivities on measured pressure values obtained from actual field data.
In view of the results obtained in section 3, we shall use updating on this test case.

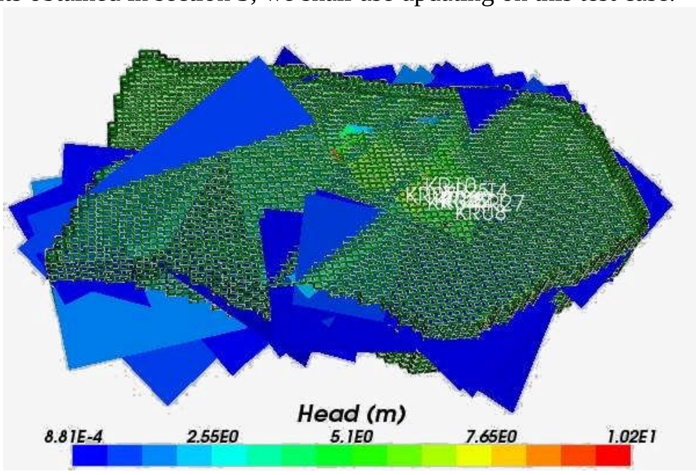

Figure 2. Domain of the large scale test case.

4.1 – CONDITIONING ON ARTIFICIAL PRESSURE VALUES

The fracture geometry and transmissivities in this test case are based on data from a real site and have been put into the model deterministically. We want to be able to test our proposed conditioning algorithm on this test case when we know a solution exists. To do this, we generate four sets of random target transmissivities. Each set will produce different target pressures at the measurement points which we shall call the “artificial” pressure measurements. The original unconditioned transmissivities based on test site data are used as initial transmissivity values. We condition these initial transmissivities on the different sets of “artificial” pressure measurements. Note that the geometry of the fractures is not changed. The sets of target transmissivities were generated from a log-normal distribution of

$$P(T) = \frac{1}{\sigma\sqrt{2\pi}T} e^{-(\ln T - M)^2/(2\sigma^2)}, \qquad (17)$$

where T is the transmissivity, M is the mean of the logarithm of T and σ is the standard deviation of the logarithm of T.

Four different sets of fracture transmissivities for the 501 fractures have been generated using different mean transmissivities μ and standard deviations sd of the associated normal distribution of the transmissivities; thus, $M = \log(\mu)$ in equation (17). These values are shown in Table 3 for the four different fracture sets.

Case	μ	sd
A	2e-6	1e-6
B	2e-5	1e-6
C	2e-3	1e-6
D	2e-5	1e-3

Table 3. The mean transmissivity value and standard deviation of the associated normal distribution of the fracture transmissivities for the four generated fracture sets.

Figure 3 shows the "artificial" measured pressure values at each measurement point corresponding to each of the cases above compared to the unconditioned pressures. Cases A, B and C are close to the unconditioned pressure values; case D differs by a greater amount. Note that there is no conditioning involved in Figure 3.

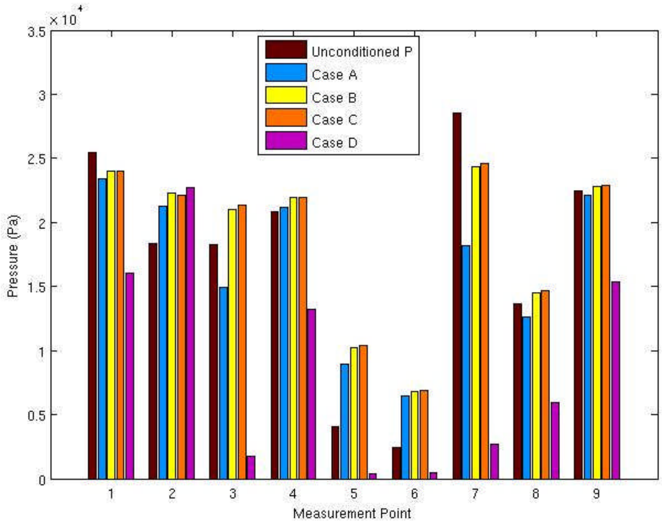

Figure 3. Pressure values at each measurement point for the unconditioned transmissivities and the 4 cases of randomly generated transmissivities from log-normal distributions.

The transmissivity values corresponding to the unconditioned pressures were used as initial transmissivities. These were then conditioned using the pressures from the four different cases as measured pressure values.
The conditioning method managed to agree exactly with the pressure values calculated in cases A, B and C. The conditioning method does not agree exactly with the pressures obtained from case D, but gives a close approximation. Figure 4 shows the "artificial" measured pressures obtained from each of the cases compared to the conditioned pressure at each measurement point. Table 4 shows the initial error measure and initial relative error, final error measure and final relative error and the number of Levenberg Marquardt iterations required for each of the cases. We define the relative error as

$$\text{Relative Error} = \frac{1}{\mathrm{m}} \sum_{\mathrm{m}} \frac{|P_{\mathrm{calc}} - P_{\mathrm{meas}}|}{P_{\mathrm{meas}}}, \qquad (18)$$

for the m measurement points.

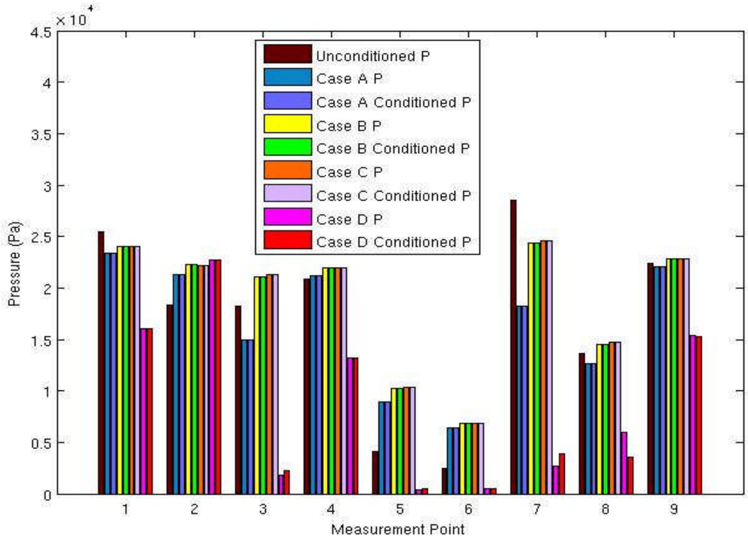

Figure 4. Conditioned pressure values compared to the "artificial" measured pressure values corresponding to each test case set of transmissivities for each measurement point.

Case	Initial Error Measure	Final Error Measure	Initial Relative Error	Final Relative Error	Number of Iterations
A	1.70638e8	0.29	0.25424	0	10
B	1.02515e8	0.47	0.20889	0	9
C	1.04162e8	0.12	0.21532	0	10
D	1.23318e9	7.43278e6	4.12383	0.19146	24

Table 4. The initial error measure, the final error measure, the initial relative error, the final relative error and the number of iterations of the Levenberg Marquardt algorithm required to converge to the final error, shown for each of the generated transmissivity cases with updating.

4.2 – CONDITIONING ON MEASURED PRESSURE VALUES

In this section we use the same initial fracture transmissivities and geometry as in section 4.1, but now we employ measured pressure values at each borehole obtained from field measurements. If ConnectFlow is used to calculate pressures at the boreholes using the unconditioned set of fractures with initial values of transmissivities, the computed pressures clearly do not agree with the measured values. Our aim is to determine fracture transmissivities that lead to calculated pressure values that are a close match to the observed pressures. Figure 5 compares the conditioned pressures to both the measured pressure and initial unconditioned pressure for all the measurement points. It can be seen that the conditioned pressures give a closer match to the measured pressure at every measurement point compared to the unconditioned pressures but do not give an exact match. Figure 6 plots the error measure against the iteration of the Levenberg-Marquardt method, while Table 5 shows the initial and final error measure and relative error between the calculated pressures and the measured pressure values.

The geometry of the fracture network is fixed and it is only the fracture transmissivities that are updated to fit the measured pressures. There is no guarantee that a solution exists to match the pressure measurements with this fracture geometry. The conditioned pressure values may well be the best agreement to measurements possible with this fracture geometry. The match to measured pressures may also be affected by inaccurate boundary conditions. On the other hand, with 501 parameters being changed to agree with 9 measurement values there will be many local minima. During the optimisation process the Levenberg-Marquardt method may well converge to one of these minima.

Initial Error Measure	Final Error Measure	Initial Relative Error	Final Relative Error
1.2731e10	3.8847e9	0.6828	0.3574

Table 5. The initial error measure between the measured pressures and the unconditioned pressures, the final error, the initial relative error and the final relative error.

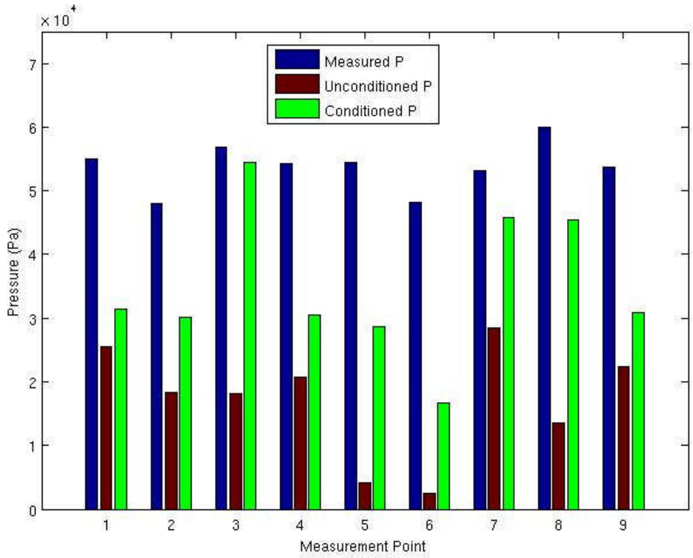

Figure 5. The measured pressures, unconditioned pressures, and conditioned pressures for the nine measurement points.

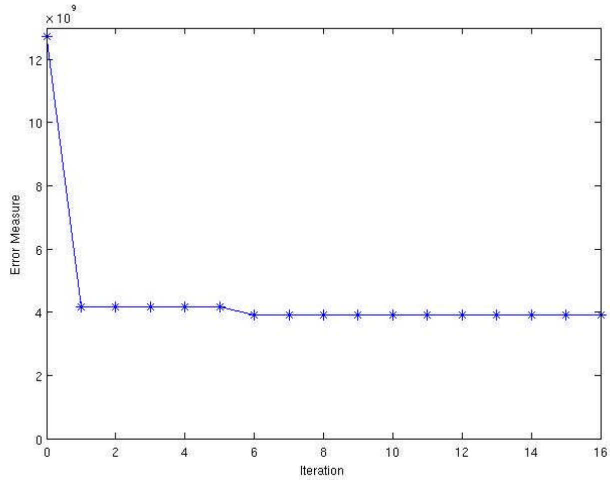

Figure 6. Error measure against iteration of the Levenberg-Marquardt method.

We considered two techniques to help the method to overcome local minima. Firstly, we aimed to improve the match to the measured pressures by using the set of fracture transmissivities that produced the conditioned pressures in Figure 5 as initial transmissivity values.
Thus the method was starting from the local minimum that may have previously been found. With these conditioned transmissivities we restarted the whole conditioning process (recalculate adjoints, sensitivities, perform Levenberg-Marquardt method etc.). A slight improvement was found with a new error measure of 2.77523e9 but there was no significant change in the match to the measured pressures.
A possible way of improving the match to the measured pressures would be to use a homotopy method. This involves changing the values of the measured pressures within the range between the unconditioned and measured pressures in Figure 5. To this end, the conditioning code is first run conditioning on pressures close to the unconditioned pressures. A final value of weights from this run

are then obtained. The code is then run conditioned on pressures further away from the initial unconditioned pressures; this results in a new set of weights. The process continues running the code, conditioned on pressures approaching the measured values, with new weights obtained at each step. However, we found that this homotopy method does not improve the overall accuracy of the conditioning method.

5 – SUMMARY AND CONCLUSIONS

We have developed a new conditioning method for fracture networks based on previous work undertaken on continuous porous media. The practical driver for the work is the need to reproduce measurements of pressure in a fracture network based on limited measurement points. Our conditioning method conditions fracture transmissivities on measured pressure values. The proposed conditioning method was tested on a number of simple test cases. The conclusions taken from these simple test cases were that updating of the derivatives (13) and (14) from the Levenberg Marquardt method should be employed in order to improve the robustness of the conditioning method. It was apparent that the convergence of the method is dependent on the geometry of the fractures and the boundary conditions employed.

Furthermore, the conditioning method was used on a test case based on data from a real test site consisting of 501 fractures with 9 measured pressure values. Firstly, "artificial" pressure values obtained from generated sets of fracture transmissivities were used to condition the initial fracture transmissivities; the geometry of the fractures was not changed. Four different cases were studied, each with different target fracture transmissivities. The resulting pressures for the four cases were used as "artificial" measured pressures that were conditioned on. The conditioning method gave an exact agreement with the "artificial" measured pressures for three of the cases and a close but not exact agreement in the fourth test case, where the transmissivity distribution had a larger variance. Finally, the fracture transmissivities were conditioned on measured pressures from field data. The conditioning gave a considerable improvement to the calculated pressure at every measurement point but failed to agree exactly with the measured pressure values. There are many potential reasons why the conditioned pressures in our practical test case do not exactly match the measured pressures. Indeed, the lack of agreement to measured values may occur because the initial 501 fracture transmissivity values may not be sufficiently close to the solution transmissivities which yield the measured pressures. This could result in the Levenberg Marquardt method converging to a local minimum. Another explanation for the lack of agreement to measured values is that the geometry of the fracture network could be incorrect. With our fixed fracture geometry there is no guarantee that a solution exists that will give the measured pressure values. Additionally, when studying large fracture networks boundary conditions should be carefully prescribed to ensure that the model is as accurate as possible. These areas of uncertainty form part of our future programme of research.

REFERENCES

[1] E. Bonnet, O. Bour, N.E. Odling, P. Davy, I. Main, P. Cowie, and B. Berkowitz, Scaling of fracture systems in geological media Reviews of Geophysics 39 (2001) 36.

[2] J. Carrera, A. Alcolea, A. Medina, J. Hidalgo, and L.J. Slooten, Inverse problem in hydrogeology. Journal of Hydrogeology 13 (2005) 16.

[3] O.A. Cirpka, and P.K. Kitanidis, Sensitivity of temporal moments calculated by the adjoint-state method and joint inversing of head and tracer data. Advances in Water Resources 24 (2000) 89-103.

[4] K.A. Cliffe, and C.P. Jackson, A New Method for Conditioning Stochastic Groundwater flow Models on Head Data, AEA Technology, Harwell, 2000.

[5] P.M. Clifton, and S.P. Neuman, Effects of Kriging and Inverse Modelling on Conditional Simulation of the Avra Valley Aquifer in Southern Arizona. 1982 18 (1982) 1215-1234.

[6] R.L. Cooley, A comparison of several methods of solving nonlinear-regression groundwater flow equations. Water Resources Research 21 (1985) 1525-1538.

[7] Z. Dai, and J. Samper, Inverse problem of multicomponent reactive chemical transport in porous media: Formulation and applications. Water Resources Research 40 (2004).

[8] G.E. Grisak, and J.F. Pickens, Solute Transport Through Fractured Media, 1, The Effect of Matrix Diffusion. Water Resources Research 16 (1980) 719-730.
[9] L. Hartley, NAPSAC Technical Summary, Version 9.3, Serco Technical Services, 2000.
[10] A.F. Hernandez, S.P. Neuman, A. Guadagnini, and J. Carrera, Inverse stochastic moment analysis of steady state flow in randomly heterogenous media. Water Resources Research 42 (2006).
[11] P.S. Huyakorn, B.H. Lester, and C.R. Faust, Finite Element Techniques for Modelling Groundwater Flow in Fractured aquifers. Water Resources Research 19 (1983) 1019-1035.
[12] K. A. Cliffe, and C.P. Jackson, Conditioning stochastic groundwater flow models on head data. Materials Research Society Symposium Proceedings 353 (1995) 7.
[13] R. Marrett, Aggregate properties of fracture populations. Journal of Structural Geology 18 (1996) 9.
[14] A. Medina, and J. Carrera, Coupled estimation of flow and solute transport parameters. Water Resources Research 32 (1996) 3063-3076.
[15] A. Milne, Topics in Flow in fractional Media, Mathematical Sciences, University of Nottingham, 2010.
[16] S.P. Neuman, Calibration of Distributed Parameter Groundwater Flow Models Viewed as a Multiple-Objective Decision Process under Uncertainty Water Resources Research 9 (1973) 1006-1021.
[17] S.P. Neuman, A Statistical Approach to the Inverse Problem of Aquifer Hydrology 3. Improved Solution Method and Added Perspective. Water Resources Research 16 (1980) 331-346.
[18] S.P. Neuman, G.E. Fogg, and E.A. Jacobson, A Statistical approach to the Inverse Problem of Aquifer Hydrology: 2. Case Study. Water Resources Research 16 (1980) 33-58.
[19] W.H. Press, B.P. Flannery, S.A. Teukolsky, and W.T. Vetterling, Numerical Recipes, Cambridge, 1986.
[20] D.T. Snow, The frequency and apertures of fractures in rock. Rock Mechanics and Mineral Sciences 7 (1970) 23-40.
[21] R.W. Zimmerman, and G.S. Bodvarsson, Hydraulic Conductivity of Rock Fractures. Transport Porous Media 23 (1996) 30.